MOP-6827

TITLE: PROCEDURES FOR OP-FTIR CONCENTRATION DATA ANALYSIS USING *IMACC FTIR SOFTWARE SUITE*

SCOPE: This procedure details the initial processing of raw OP-FTIR data. The outputs of the following procedure are path-integrated concentrations (PIC) of the particular compound(s) of interest. These PIC values may be used as input to the Radial Plume Mapping (RPM) algorithms described in MOPs 6841, 6842 and 6843. The following procedure is for performing analysis with the *IMACC FTIR Software Suite*,* using data collected by IMACC, RAM2000, or Midac OP-FTIR systems.

PURPOSE: To provide an overview of how to perform the analysis on OP-FTIR data from different instruments, using the *IMACC FTIR Software Suite* to create either PICs or Path-Averaged Concentrations (PACs).

1.0 DATA FILE FORMAT AND ORGANIZATION

1.1 Data-File Path Organization

When measuring over multiple paths, the measurement-data files should be sorted into subdirectories (subfolders), with one subdirectory for each path. In addition, the data files should have file names that are indexed chronologically. *Omnic* software and some utilities have problems dealing with file paths that have spaces, so to be safe, it is best to eliminate spaces from the file and subdirectory names.

1.2 The *IMACC Software* and Utilities for Performing Post-Measurement Chemical Quantitative Analysis

The IMACC Software Suite program, *IMACC Quantify*, is the Classical Least Squares (CLS) analysis program that is used to perform post-measurement chemical analysis. In addition to this program, there are three utilities that are very useful for preparing the interferograms or spectra to input into *IMACC Quantify*. Table 1 lists the program and the utilities necessary for file preparation. The utilities can be used to prepare files for analysis and perform tasks that include: inserting data-collection information in the data-file headers; averaging spectra; creating synthetic backgrounds; and converting the file types. The *IMACC Quantify* chemometric program operates

* In addition to the *IMACC FTIR Software Suite*, there are two other chemometric software packages that are used to convert raw interferogram data to chemical path-integrated concentrations, *RMMSoft* and *Non-Lin*.

on either Omnic-SPA formatted files or Grams-SPC single files in batch mode on all single-beam or absorbance spectra that are stored in a subfolder.

Table 1. List of Software and Utilities that are used to Perform Chemical Quantification with the *IMACC FTIR Software Suite*.

Software/Utility	Location	Tasks
IMACC Quantify	IMACC Software Suite	CLS Analysis
SpaAverage	IMACC Software Suite/Tools	Set Parameters in Header, Coadd Spectra
ImaccSynthIo	IMACC Software Suite/Tools	Create Synthetic Background
ARCADIS CAOS	CAOS(version)	Convert Grams-spc to Omnic-spa Convert I-Grams to Single-Beams or Absorbances Convert Single-Beams to Absorbances Average Spectra – Running Average or Straight Average

1.3 The Requirements on the Spectral Data Input to *IMACC Quantify*

ARCADIS and EPA use three different OP-FTIR systems in their field projects: Midac, RAM2000, and IMACC. Each of these systems output the measurement data in different formats. The treatment of the measurement data from each of these systems will be described separately, followed by a table that summarizes the processing of data collected by all three instruments.

1.3.1 Midac Data Files

Until recently, the Midac data files were in standard Grams SPC format. The EPA Midac that was refurbished by Midac in 2004 was altered to create data files in a Midac proprietary multifile format. The new format uses the filename chosen by the user and appends an index with leading zeros to the file name. The suffix indicates the spectral type. For instance, if the user chooses the name R5 (for the fifth mirror), then the first few measured interferograms would have the following names: R500000001.ifg, R500000002.ifg, and R500000003.ifg. The nomenclature for the 3-character suffices are given in Table 2.

Table 2. File Nomenclature for Data Collected by Midac.

File Type	File Name
Interferogram	FileName.ifg
Single Beam	FileName.sgl
Absorbance	FileName.abs

Midac altered the format of the interferograms so that programs and utilities that work with *GRAMS/AI* format no longer work with the new Midac format. Therefore, while it is still important

to archive the primary interferogram data, in order to be analyzed by *IMACC Quantify*, the data must first be converted to single beams or absorbances. It is most expeditious to perform this conversion at the time of data collection, by choosing the option in the Midac data-acquisition software to collect both in interferograms and single beams.

The Midac formatted single-beam and absorbance data files must be converted to either GRAMS/AI-SPC or Omnic-SPA format using the ARCADIS CAOS utility. If there is no compelling reason to perform the analysis on absorbance files, it is better to perform the analysis with single beams. When performing analysis with single beams, one has the flexibility of choosing a variety of different backgrounds for different types of analyses. The operation of CAOS is described in Sections 2.2, 2.3, and 2.4.

1.3.2 RAM2000 (and Old Midac Format) Data Files

The RAM2000 analytical software package, *RMMSoft*, has a data acquisition routine that automatically saves all collected interferograms in the military-based IDA multifile format as *.dat. *RMMSoft*, has a post-measurement option to convert the IDA multifiles to Grams formatted SPC multifiles. However, the IMACC and ARCADIS utilities cannot correctly convert Gram-formatted interferograms into single-beam or absorbance spectra.

Using options in *RMMSoft*, the RAM2000 data files must be converted to single-beam or absorbance spectral files in Grams SPC format. The user has the option to convert the RAM2000 files to SPC multifiles or single files. Multifiles are easier to handle and transfer from one computer to another, or to a data storage medium. However, prior to performing the analysis, the single beam or absorbance multifiles must be converted to single files. Either *RMMSoft* may be used for this task or *GRAMS/AI* may be used, following the procedure described in Section 2.1.

If there is no compelling reason to perform the analysis on absorbance files, it is better to perform the analysis with single beams. When performing the analysis with single beams, there are a variety of different backgrounds that can be chosen for different types of analyses.

1.3.3 IMACC Data Files

The IMACC data files are in Omnic SPA format. The file nomenclature uses a time stamp for the file name and indicates the file type in the three-character suffix. This nomenclature is illustrated in Table 3.

Table 3. File Nomenclature for Data Collected by IMACC on May 26, 2004.

File Type	File Name
Interferogram	2004-05-26_154512.ifg
Single Beam	2004-05-26_154512.sgl
Absorbance	2004-05-26_154512.abs

IMACC Quantify and the IMACC/ARCADIS utilities accept and process all IMACC file types without requiring any formatting changes.

2.0 DATA ANALYSIS PROCEDURES

At this point, the data files have been reformatted to be compatible with either *GRAMS/AI* or *Omnic*. The procedures described in this section involve final manipulations of the data prior to performing the chemical analysis using *IMACC Quantify*. It is necessary to convert any SPC multifiles to SPC single files, as described in Section 2.1. Section 2.2 details the procedure for determining if a correction for stray light may be required, and how to make this correction, if necessary.

2.1 Splitting Multifiles into Single Files

Data filed in SPC multifiles format must be split to individual single files, with the output in a unique subdirectory. Since Midac no longer collects data in SPC multifiles format, this is only an issue with RAM2000 and old Midac data.

In the *GRAMS/AI* software program, from the "Applications" menu, select "AB Program..."

1. In the "Array Basic Programs" window that appears, select "MFUTILS.AB."
2. In the "GRAMS Multifile Operations" window, select "Split into Singles."
3. If no multifile is open, then a "Select Multifile to Split into Single Files" window will appear. Select the correct multifile to split.
4. When the "Filename for SAVE" window appears, select "New Filename," detail the appropriate directory, and give a name to the individual subtraction files to be created. The new files are placed in the "subsb" subdirectory, and named according to the spatial orientation and mirror appropriate to the data, keeping in mind that *GRAMS/AI* is responsible for numbering the new files consistent to their original designations (e.g., "rada_m1_00" for the separate files containing information from mirror 1 in radial scan A).
5. In the "Range Setup" window, confirm that the default settings correspond to the specifics of the raw data. For example, if there were 15 raw data files, confirm that number, and that the "First File Number" is "1" and the "Last File Number" is "15."
6. Click "OK," and *GRAMS/AI* will place the individual single beam files, with the stray light subtracted, into the designated directory.

2.2 Stray Light

Stray light is a portion of the outgoing infrared light that is scattered off of surfaces, inside the instrument enclosure, that are in the detector's field of view. Since this scattered light has not traversed the measured path, it contains none of the absorption bands of the species that are being measured. Stray light is a problem peculiar to monostatic systems and occurs more in the Midac system than in RAM2000 and IMACC. Both RAM2000 and IMACC were engineered to minimize

the internal scatter of the modulated light to the detector, whereas Midac was not. Actually, the IMACC monostatic OP-FTIR usually experiences so little stray light that one cannot collect an interferogram without using a mirror.

An easy test can be performed to determine if the stray light may be negligible. Aim the OP-FTIR to a mirror and verify that it is measuring interferograms. Then, either aim the OP-FTIR away from the mirror or remove the mirror from the field of view of the OP-FTIR. If the system no longer collects interferograms, the scatter is too weak for the system to detect the centerburst and, therefore, the internal scatter is negligibly weak.

If the quality assurance procedures in MOP-6802, Section 1.3.7 (conducted during the pre-deployment QA procedures) indicate that the quantity of stray light detected was greater than five percent, then either correct for the stray light, or state the resulting error.

2.2.1 Correction of Single-beam Files for Stray Light

The ARCADIS CAOS utility has recently been upgraded to automatically perform the stray light correction to single beam files from any of the three types of instruments. The procedure is as follows:

1. Open CAOS.
2. Go to the “Post Collect Processing” page.
3. Select “List Files” tab.
4. Select “File Extension for Process” (SPA, SPC, SGL, or SB).
5. On “Directory Main,” select “Folder” button to select the folder that contains the single-beam spectra. Click on “Select Cur Dir.” All of the files should appear in the window on the left. If no files show, check that the “File Extension for Processing” corresponds to the contents of the chosen folder.
6. In the window showing “Selected Files,” choose “All Files in the Directory.”
7. Click on “Add.” All the files should now be listed in the window on the lower right.
8. Click on the green “Start” button. The File Header Information for SPA files will be read. This may take a minute or two for larger numbers of input files.
9. Select the “Spectral Subtraction” tab.
10. Click on the “Subtrahend Filename” browse button and browse to the 16-minute, 8-cm^{-1} resolution, stray-light single-beam file.
11. Select either SPA (recommended) or SPC in the “File Extn. For” saving window.

12. Input the resolution of the measurement single beams into the resolution window.

13. Click on the green "Go" button. The converted files will automatically be saved to a new subdirectory (attached to the data-file directory) named "Stray-Light Corrected." These files are not only corrected, but they are now in a format that can be processed by *IMACC Quantify*.

2.3 Spectral Averaging

In some cases, such as when measuring short-term phenomena, the collection time may be short. The signal-to-noise on spectra improves with the square-root of the measurement time. Therefore, in these sort of cases, the detection limits may be too high to detect some of the target chemical species. The detection limits can be lowered by averaging the spectra. The ARCADIS CAOS utility performs this task to produce either straight averages or running averages. An example would be to convert 10-second averaged data to 30 seconds by performing a 3-point average, or to 60 seconds by performing a 6-point average.

2.3.1 Procedure for Spectral Averaging

The procedure for averaging spectra is as follows:

1. Open CAOS.

2. Go to the "Post Collect Processing" page.

3. Select "List Files" tab.

4. Select "File Extension for Process" (SPA, SPC, SGL, SB, or ABS).

5. On "Directory Main," select "Folder" button to select the folder that contains the single-beam spectra. Click on "Select Cur Dir." All of the files should appear in the window on the left. If no files show, check that the "File Extension for Processing" corresponds to the contents of the chosen folder.

6. In the window showing "Selected Files," choose "All Files in the Directory."

7. Click on "Add." All the files should now be listed in the window on the lower right.

8. Click on the green "Start" button. The File Header Information for SPA files will be read. This may take a minute or two for larger numbers of input files.

9. Select the "Spectral Average" Tab.

10. Choose the "Number of Spectra to Average." If a running average is desired, press the "Moving Average" button.

11. Select either SPA (recommended) or SPC in the "File Format for Average" window.

12. Click on the green "Go" button. The converted files will be automatically saved to a new subdirectory (attached to the data-file directory) named "Average." These files are now ready to be processed by *IMACC Quantify*.

2.4 File Format Conversion

Stray-light correction, spectral averaging, or any other procedure performed by ARCADIS CAOS will output the files as either SPC or SPA for input into *IMACC Quantify*. All data file types collected by IMACC, *.ifg, *.sgl, and *.abs, do not require conversion. However, for data collected by other systems that are not in SPC format (as would be the case for data collected by Midac), the file conversion must be performed prior to the analysis. This procedure can also be used to convert SPC to SPA, or vice versa.

2.4.1 Procedure for File Conversion to SPC or SPA Formats

The ARCADIS CAOS utility has recently been upgraded to automatically perform the stray light correction to single beam files from any of the three types of instruments. The procedure is as follows:

1. Open CAOS.

2. Go to the "Post Collect Processing" page.

3. Select "List Files" tab.

4. Select "File Extension for Process" (SPA, SPC, SGL, SB, or ABS).

5. On "Directory Main," select "Folder" button to select the folder that contains the single-beam spectra. Click on "Select Cur Dir." All of the files should appear in the window on the left. If no files show, check that the "File Extension for Processing" corresponds to the contents of the chosen folder.

6. In the window showing "Selected Files," choose "All Files in the Directory."

7. Click on "Add." All the files should now be listed in the window on the lower right.

8. Click on the green "Start" button. The File Header Information for SPA files will be read. This may take a minute or two for larger numbers of input files.

9. Select the "Reprocess" tab.

10. Choose single beam or absorbance as the "Final Format." If single beams are being converted to absorbance, select the appropriate background by clicking on the "Folder" button to initiate browsing.

11. Select either SPA (recommended) or SPC in the "File Format for Average" window.

12. Input the resolution of the measurement single beams into the resolution window.

13. Click on the green "Go" button. The converted files will be automatically saved to a new subdirectory (attached to the data-file subdirectory) named either "Singlebeams" or "Absorbances." These files are now ready to be processed by *IMACC Quantify*.

2.5 *IMACC Quantify*

IMACC Quantify is a comprehensive chemical analysis software package that has a very large degree of flexibility. The software performs a CLS analysis with baseline-bias and -slope correction. The software can correct for local temperature, barometric pressure (important at high altitudes), frequency shift, spectral non-linearity, and spectral bias. The *IMACC Quantify* software provides many different options and methods of optimizing the analysis. With this degree of complexity, it is best to refer the user to the *IMACC Quantify* User's Manual and point out some of the unique issues relating to analyzing EPA data that are not covered in the manual.

All of the calculated concentrations and standard errors are given in path-averaged units of ppm. If PIC determinations are desired, one must specify that the pathlength is one meter, in the "Batch Directory" window.

Another issue that will occur with EPA data relates to the requirement that sample spectra, the background spectra, the frequency-shift reference, the bias reference set, the spectral calibration references, and the linearity spectral sets all have identical data-point spacing. Unfortunately, Midac, RAM2000, and IMACC all collect spectral measurements with different data-point spacings. To mix and match references from different sources, all of the data must have the same data-point spacing. There are two methods of matching the data-point spacings, one for spectra in GRAMS/AI-SPC format and one for IMACC-SPA format.

2.5.1 Spacing Correction to Match IMACC Format

This procedure must be followed for any SPC or SPA formatted spectra that are to be analyzed using the standard IMACC data-point spacing.

1. Open *Omnic*.

2. Open the SPC or SPA formatted spectrum (*Omnic* can open SPC formatted spectra).

3. Select "Change Data Spacing" in the "Process" menu.

4. Select a data spacing value that is one half the resolution. For instance, if the resolution of the field measurements is 0.5 cm^{-1}, select a data-spacing value of 0.25.

5. Save the corrected spectrum as either an SPC or SPA file.

2.5.2 Spacing Correction to Match SPC Format

The data in SPC format will have different data-point spacing, depending on whether the data was collected by the new Midac or RAM2000 (and old Midac). The data-point spacing of the samples (and background) can be matched to the references, or vice versa. The procedure is as follows:

1. Open *Grams*.

2. Open a "template" spectrum (a spectrum which has the desired data-point spacing) to occupy Slot # 1.

3. Open the spectrum on which the spacing is to be corrected to occupy Slot #2. The spectra to be spacing-corrected can be either in multifiles or in single files. If many single files need to be corrected, additional files can be opened to occupy Slots #3, #4, etc. After this has been done, use "Page Up" or "Pahe Down" to select Slot #2 in the window.

4. Press "Control / k" to activate the interactive calculator.

5. Enter the equation, #s=intrp(#1,#s), and click on "Execute" and then "Done." The symbol "#s" refers to the selected "sample," which now is in Slot #2.

6. If there are more files to be corrected (in Slots #3, #4, etc.) page down to Slot #3 and repeat Steps 4. and 5. The interactive calculator will remember the expression that was previously entered, so just click on "Execute" and "Done." Repeat for any additional files to be corrected.

7. Save all corrected files.

3.0 ASSESSMENT OF THE ACCURACY OF THE PIC MEASUREMENTS

Upon completion of the data analysis process, the accuracy of the PIC measurements should be evaluated by examining the analyzed nitrous oxide concentrations. The nitrous oxide concentrations should be 315 ppb ± 25% for pathlengths less than 50 meters, 315 ppb ± 15% for pathlengths between 50 and 100 meters, and 315 ppb ± 10% for pathlengths greater than 100 meters. If the analyzed nitrous oxide concentrations do not meet these acceptance criteria, the data should be re-processed using different designated boundaries.

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